



chain nodes :

13 14 15 16 17 18 19 20 21 22 23 24 26 91 92 93 94 95 96 97 98 99 100
102 103 104 105 106 107 109 110 112

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 27 28 29 30 31 32 33 34 35 36 37 38 39 40
41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64
65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80

chain bonds :

1-16 1-20 2-15 2-19 3-13 3-18 5-22 5-23 6-17 6-21 12-24 13-14 23-112 24-26 32-91
38-92 44-93 50-94 56-95 62-96 68-97 74-98 80-99 91-104 92-105 93-106 94-107 95-109
96-110 97-100 98-102 99-103

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 27-28 27-32 28-29 29-30
30-31 31-32 33-34 33-38 34-35 35-36 36-37 37-38 39-40 39-44 40-41 41-42 42-43
43-44 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56
57-58 57-62 58-59 59-60 60-61 61-62 63-64 63-68 64-65 65-66 66-67 67-68 69-70
69-74 70-71 71-72 72-73 73-74 75-76 75-80 76-77 77-78 78-79 79-80

exact/norm bonds :

1-2 1-6 1-16 2-3 2-15 3-4 4-5 5-6 5-23 6-17 23-112 24-26 91-104 92-105 93-106
94-107 95-109 96-110 97-100 98-102 99-103

exact bonds :

1-20 2-19 3-13 3-18 5-22 6-21 12-24 13-14 32-91 38-92 44-93 50-94 56-95 62-96
68-97 74-98 80-99

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38
34-35 35-36 36-37 37-38 39-40 39-44 40-41 41-42 42-43 43-44 45-46 45-50 46-47
47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56 57-58 57-62 58-59 59-60
60-61 61-62 63-64 63-68 64-65 65-66 66-67 67-68 69-70 69-74 70-71 71-72 72-73
73-74 75-76 75-80 76-77 77-78 78-79 79-80

G1:Cb,Cy,Hy

G2:[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 26:CLASS 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom
52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom
62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom
72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 91:CLASS
92:CLASS 93:CLASS 94:CLASS 95:CLASS 96:CLASS 97:CLASS 98:CLASS 99:CLASS 100:CLASS
102:CLASS 103:CLASS 104:CLASS 105:CLASS 106:CLASS 107:CLASS 109:CLASS 110:CLASS
112:CLASS